

The Optimum Inverse Problem of Numerical Error Analysis

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$$\left. \begin{array}{l} \text{inputs} \\ \text{initial data} \\ y \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} \text{outputs} \\ \text{solution} \\ x \end{array} \right.$$

- Equations

$$F(y, x) = 0$$

F is the residual function.

- Solution function

$$f(y) = x$$

$$F(y_0, x_0) = 0$$

$$F(\underbrace{y_0 + \Delta y}_{y'}, \underbrace{x_0 + \Delta x}_{\bar{x}}) = 0$$

1. Is the solution mathematically stable?

$$\|\Delta x\| \leq \chi \|\Delta y\| + o(\|\Delta y\|)$$

$$\chi_{\min} = \|\mathcal{D}f(x_0)\|$$

2. Inverse Problem. What size of Δy is needed to accomodate an \bar{x} ?

A. *A priori* inverse rounding error analysis:
for any \bar{x} , construct a Δy and bound it.

$$\|\Delta y\| \leq \text{bound on backward errors}$$

B. *A posteriori* analysis

$$\begin{aligned} \mu(\bar{x}) &= \left\{ \begin{array}{l} \text{minimal} \\ \text{optimal} \\ \text{smallest} \end{array} \right\} \begin{array}{l} \text{size of} \\ \text{backward} \\ \text{errors} \end{array} \\ &= \min_{\{y' : F(y', \bar{x}) = 0\}} \|y' - y_0\| \end{aligned}$$

Examples of Minimal Size, $\mu(\bar{x}) =$

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Linear Equations, $A_0 x = b_0$ [Oettli and Prager, 64]

$$\min_{\Delta A, \Delta b} \max_{i, j, k} \left\{ \left| \frac{\Delta A_{i,j}}{E_{i,j}} \right|, \left| \frac{\Delta b_k}{f_k} \right| \right\} = \max_j \left| \frac{(A_0 \bar{x} - b_0)_j}{(|E| |\bar{x}| + |f|)} \right|$$

Linear Equations, $A_0 x = b$ [Rigal and Gaches, 67]

$$\min_{\Delta A} \|\Delta A\| = \frac{\|\bar{r}\|}{\|\bar{x}\|} \quad \text{where } \bar{r} = A_0 \bar{x} - b$$

Linear Least Squares [Waldén, Karlson, Sun, 95]

$$\min_{\Delta A} \|\Delta A\|_F = \sqrt{\frac{\|\bar{r}\|_2^2}{\|\bar{x}\|_2^2} + \min_i \left\{ 0, \lambda_i \left(A_0 A_0^t - \frac{\bar{r} \bar{r}^t}{\|\bar{x}\|_2^2} \right) \right\}}$$

Minimal Backward Error Bibliography

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linear equations	1964	Oettli, Prager	structured LE
	1967	Rigal, Gaches	LE
	1989	Bunch, Demmel, Van Loan	symmetric LE
	1991	Sun	Choleski and QR
	1992	Bartels, Higham	Vandermonde LE
various factorizations		Higham, Higham	Toeplitz LE
		Higham, Higham	multiple right side LE
	1993	Sun	characteristic subspaces
	1994	Chandrasekaran, Ipsen	sym. eigen decomp.
		Varah	Toeplitz LE
linear least squares	1995	Smoktunowicz	symmetric structured LE
		Smoktunowicz	eigenvalue and vector
		Sun	sym. eigen decomp.
		Waldén, Karlson, Sun	LLS
	1996	Higham	alt. expression for LLS
invariant subspaces		Sun	multiple right side LLS
	1997	Karlson, Waldén	estimate for LLS
		Sun, Sun	underdetermined LE
		Sun	min. norm sltn. for LLS
	1998	Frayssé, Toumazou	eigenvalue and vector
		Higham, Higham	eigenvalue and vector
		Sun	Vandermonde LE
	1999	Cox, Higham	linearly constrained LLS
		Gu	estimate for LLS
	2001	Malyshev	spherically constrained LLS
	2002	Malyshev, Sadkane	evaluation for sparse LLS
		Stewart	Krylov subspaces

1. **Accuracy criterion.** [von Neumann, 47]

If the initial data have error $\geq \mu(\bar{x})$,
then \bar{x} solves the problem,
to the extent the problem is known.

2. **Backward stability estimation.**

An \bar{x} with a small $\mu(\bar{x})$ is backward
stable.

3. **Test new algorithms.**

Explore backward stability without having
to do an inverse rounding error analysis.

1. Forward Type	2. Inverse Type	
	A. Inverse Rounding Error Analysis	B. Mathematical Analysis
<i>Find $\chi(y_0)$, the condition number.</i> $\chi_{\min} = \ \mathcal{D}f(y_0)\ $	<i>Construct some backward errors.</i>	<i>Find $\mu(\bar{x})$, the minimal size of backward error.</i> $\mu(\bar{x}) = ?$

Background

Abstract Formulation of the Problem

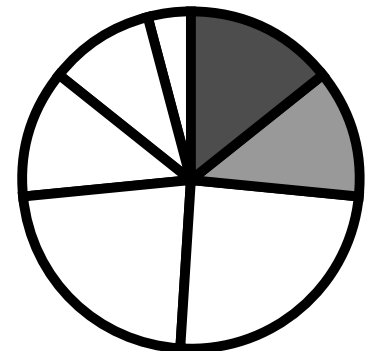
Perturbation Theory of Metric Projections

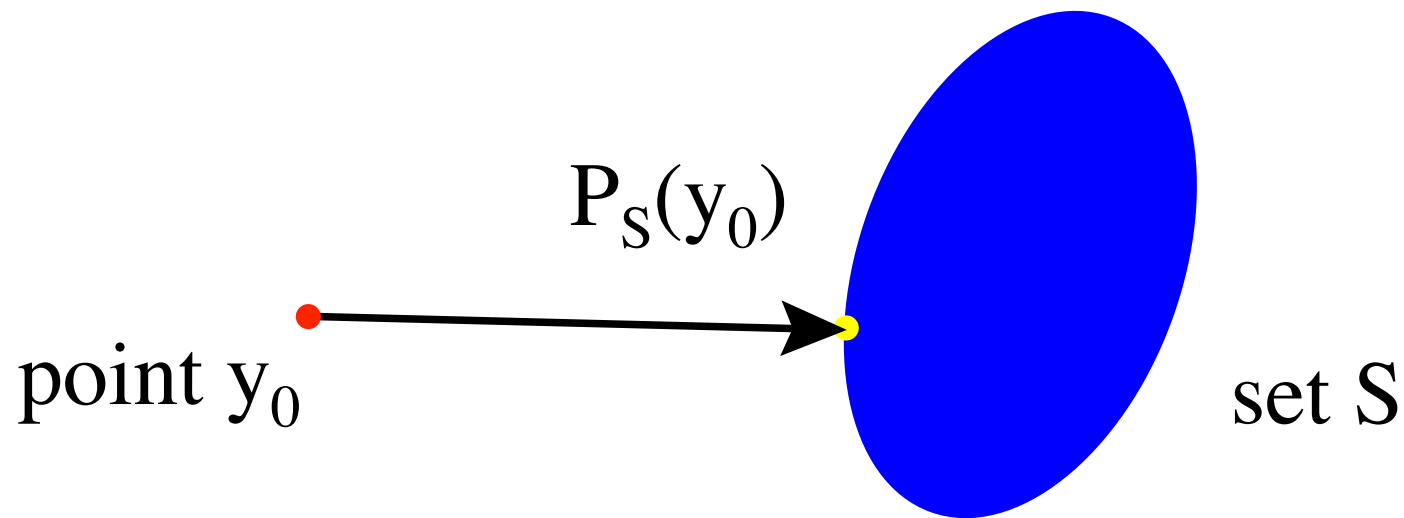
Asymptotic Approximation

Application to Linear Least Squares

Numerical Examples

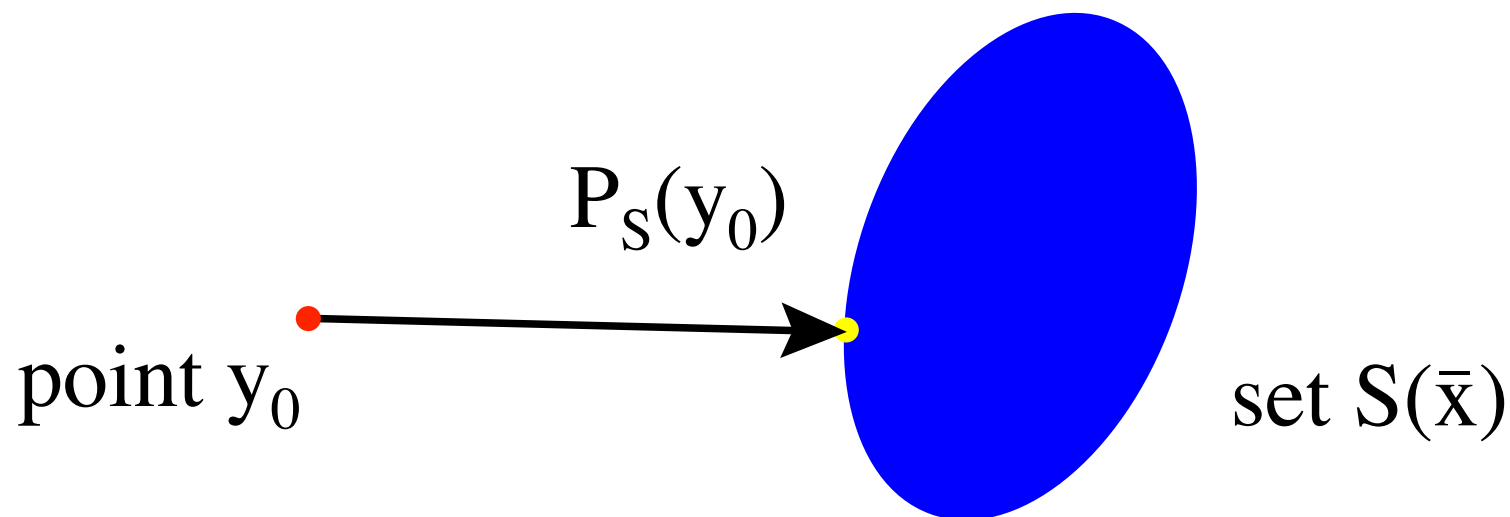
Conclusion





$P_S(y_0)$ = a point in set \mathcal{S} nearest to y_0

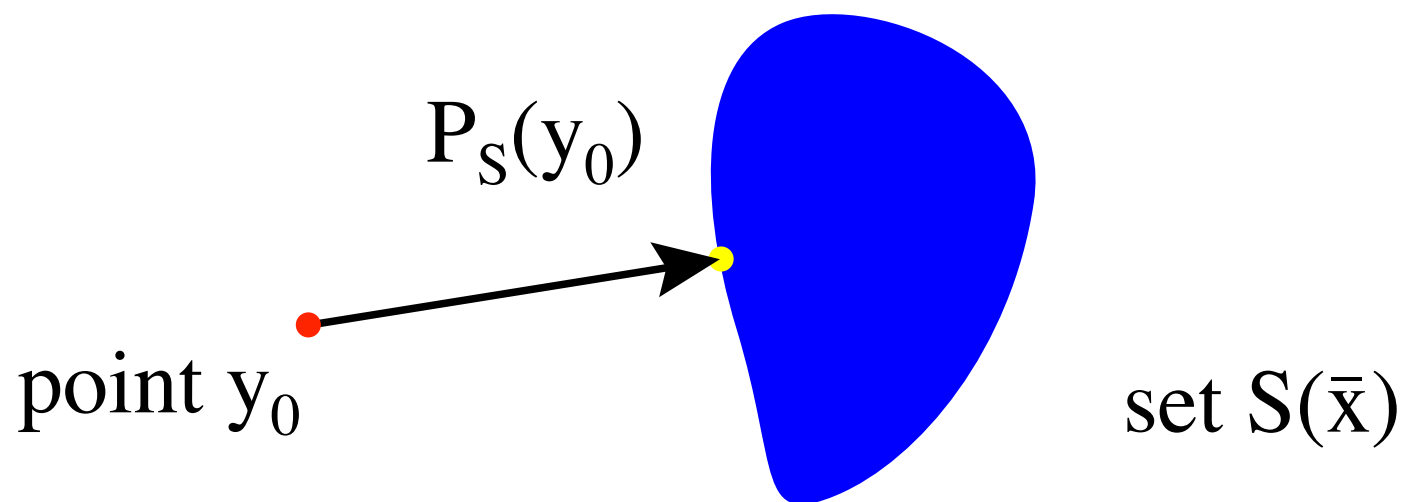
$\text{dist}(y_0, \mathcal{S})$ = distance from y_0 to \mathcal{S}



Minimal size of backward error is

$$\mu(\bar{x}) = \text{dist}(y_0, \underbrace{\{y' : F(y', \bar{x}) = 0\}}_{\mathcal{S}(\bar{x})})$$

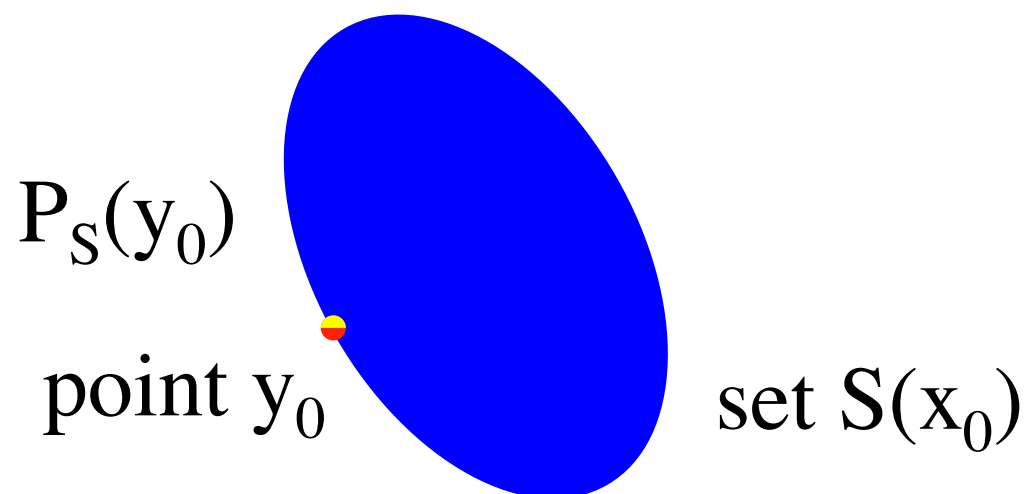
all data compatible with \bar{x}



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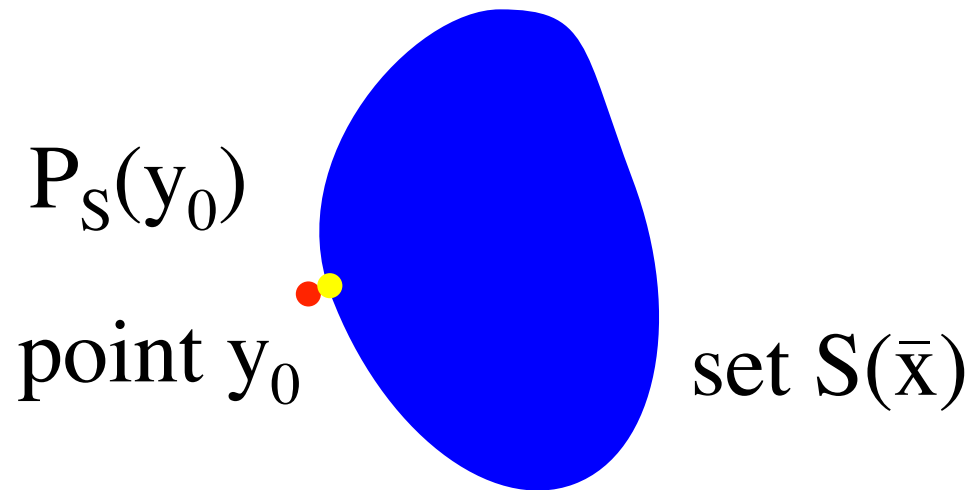
all data compatible with \bar{x}



Minimal size of backward error is

$$\mu(\bar{x}) = \text{dist}(y_0, \underbrace{\{y' : F(y', \bar{x}) = 0\}}_{\mathcal{S}(x_0)})$$

all data compatible with x_0



Minimal size of backward error is

$$\mu(\bar{x}) = \text{dist}(y_0, \underbrace{\{y' : F(y', \bar{x}) = 0\}}_{\mathcal{S}(\bar{x})})$$

all data compatible with \bar{x}

Minimal size of backward error is a distance

$$\mu(\bar{x}) = \min_{y' \in \mathcal{S}(\bar{x})} \|y' - y_0\|$$

$$\mathcal{S}(\bar{x}) = \{y' : F(y', \bar{x}) = 0\}$$

- ★ The set $\mathcal{S}(\bar{x})$ is subject to change.
- ★ The point y_0 is not subject to change.
- ★ $\bar{x} \approx x_0$, which places $\mathcal{S}(\bar{x})$ near y_0 .
- ★ The true solution x_0 is unknown.

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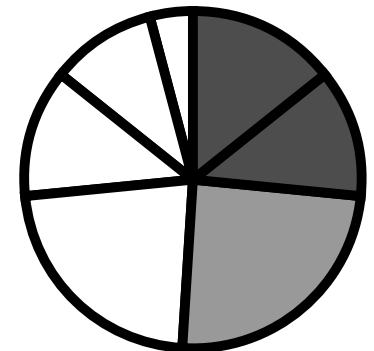
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Differentiation with respect to y_0 (not \mathcal{S}) for

$$\left\{ \begin{array}{c} \text{dist}(y_0, \mathcal{S}) \\ P_{\mathcal{S}}(y_0) \end{array} \right\} \times \left\{ \begin{array}{c} y_0 \in \mathcal{S} \\ y_0 \notin \mathcal{S} \end{array} \right\} \times \left\{ \begin{array}{c} \text{convex } \mathcal{S} \\ \text{unconvex} \end{array} \right\} \times \dots$$

$$\left\{ \begin{array}{c} \text{Hilbert space} \\ \text{Banach space} \end{array} \right\} \times \left\{ \begin{array}{c} \text{finite dimensional} \\ \infty \text{ dimensional space} \end{array} \right\} = 2^5$$

★ Basic negative result: $P_{\mathcal{S}}(y_0)$ need not be directionally differentiable everywhere in \mathbb{E}^2 for convex \mathcal{S} .

— [Kruskal, 69] [Shapiro, 94]

Differentiation with respect to y_0 (not \mathcal{S}) for

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- ★ Basic positive result: $P_{\mathcal{S}}(y_0)$ is directionally differentiable everywhere at boundary of convex \mathcal{S} in Hilbert spaces.
— [Zarantonello, 71]

1. Differentiability at internal points $y_0 \in \text{bd}(S)$:

(a) Convex S :

Hilbert spaces: $P_S(y_0)$ is directionally differentiable always.
[Zarantonello, 71]

(b) Arbitrary S :

Finite dimensional Banach spaces: y_0 and S have been characterized for which $P_S(y_0)$ is directionally differentiable
[Shapiro, 87]

2. Differentiability at external points $y_0 \notin S$:

(a) Convex S :

Banach spaces: $\text{dist}(y_0, S)$ is continuously differentiable in spaces with differentiable norms [Holmes, 73]

(b) Arbitrary S :

Hilbert spaces: sets have been classified that have uniform envelopes where $\text{dist}(y_0, S)$ is continuously differentiable
[Clarke et al., 95]

$$\phi(x) = \min_{y : G(y, x) \in \mathcal{K}} g(y, x)$$

“It is difficult to investigate the sensitivity of an optimal value whose feasible set is subject to change . . .”

[Bonnans and Shapiro, 98, 00]

Used for:

- sensitivity analysis [Fiacco and Ghaemi, 82]
- finding optimality conditions
- establishing the convergence of algorithms

Theory assumes continuous 2nd derivatives for both constraint and objective functions.

★ In Hilbert spaces [B&S, 00]

$$\lim_{t \rightarrow 0^+} \frac{\mu(x_0 + t\Delta x)}{t} = \min_{\Delta y : J_1 \Delta y + J_2 \Delta x = 0} \|\Delta y\|_2$$

- If F has continuous second derivatives,
- $[J_1, J_2] = \mathcal{D}F(y_0, x_0)$ has full row rank.

Use the result of B&S to estimate

$$\mu(\bar{x}) = \min_{\{y' : F(y', \bar{x}) = 0\}} \|y' - y_0\|_2$$

The directional derivative gives to 1st order

$$\mu(x_0 + \Delta x) = \min_{\Delta y : J_1 \Delta y + J_2 \Delta x = 0} \|\Delta y\|_2 + \mathcal{O}(\|\Delta x\|^2)$$

where $[J_1, J_2] = \mathcal{D}F(y_0, x_0)$.

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The **directional derivative** gives to 1st order

$$\mu(x_0 + \Delta x) = \min_{\Delta y : J_1 \Delta y + J_2 \Delta x = 0} \|\Delta y\|_2 + \mathcal{O}(\|\Delta x\|^2)$$

where $[J_1, J_2] = \mathcal{D}F(y_0, x_0)$.

Regarding (Directional) Derivatives of μ ...

1. Pure Math

Only perturbs y_0 — inapplicable to varying \mathcal{S} .

2. Optimization Theory

Studies perturbations to \mathcal{S} . ✓

- Shows derivative linearizes the constraint.
- Requires 2nd order differentiability. :-(
 - So only for 2-norm — drawback.
- Remainder not uniform in direction — serious.
- Formula needs Δx & x_0 — show stopper.

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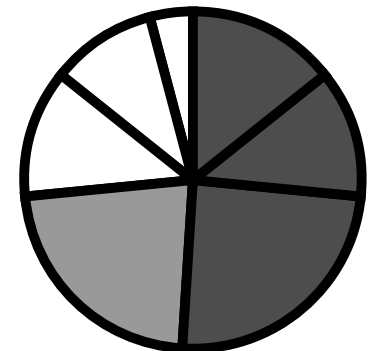
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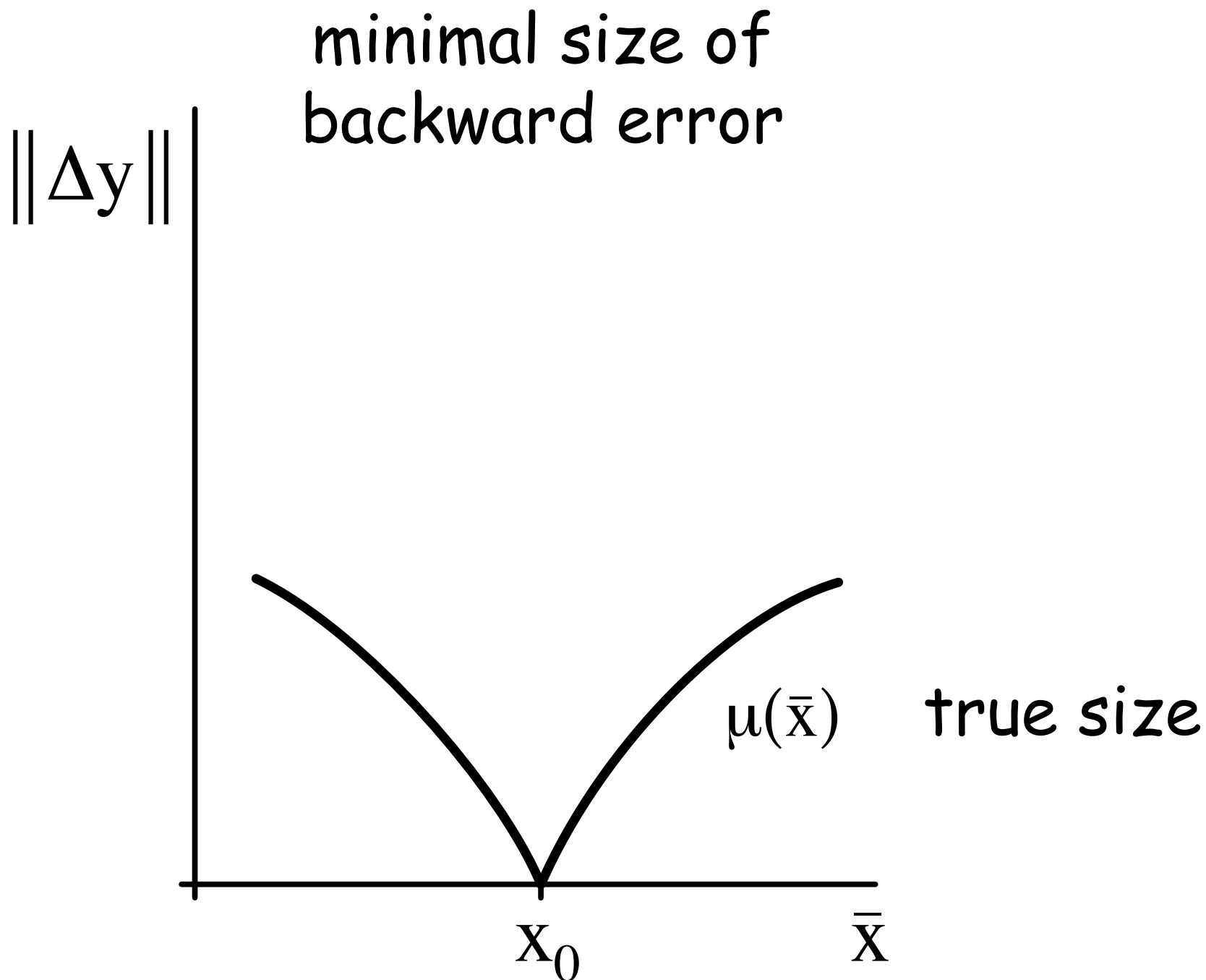
Asymptotic Approximation

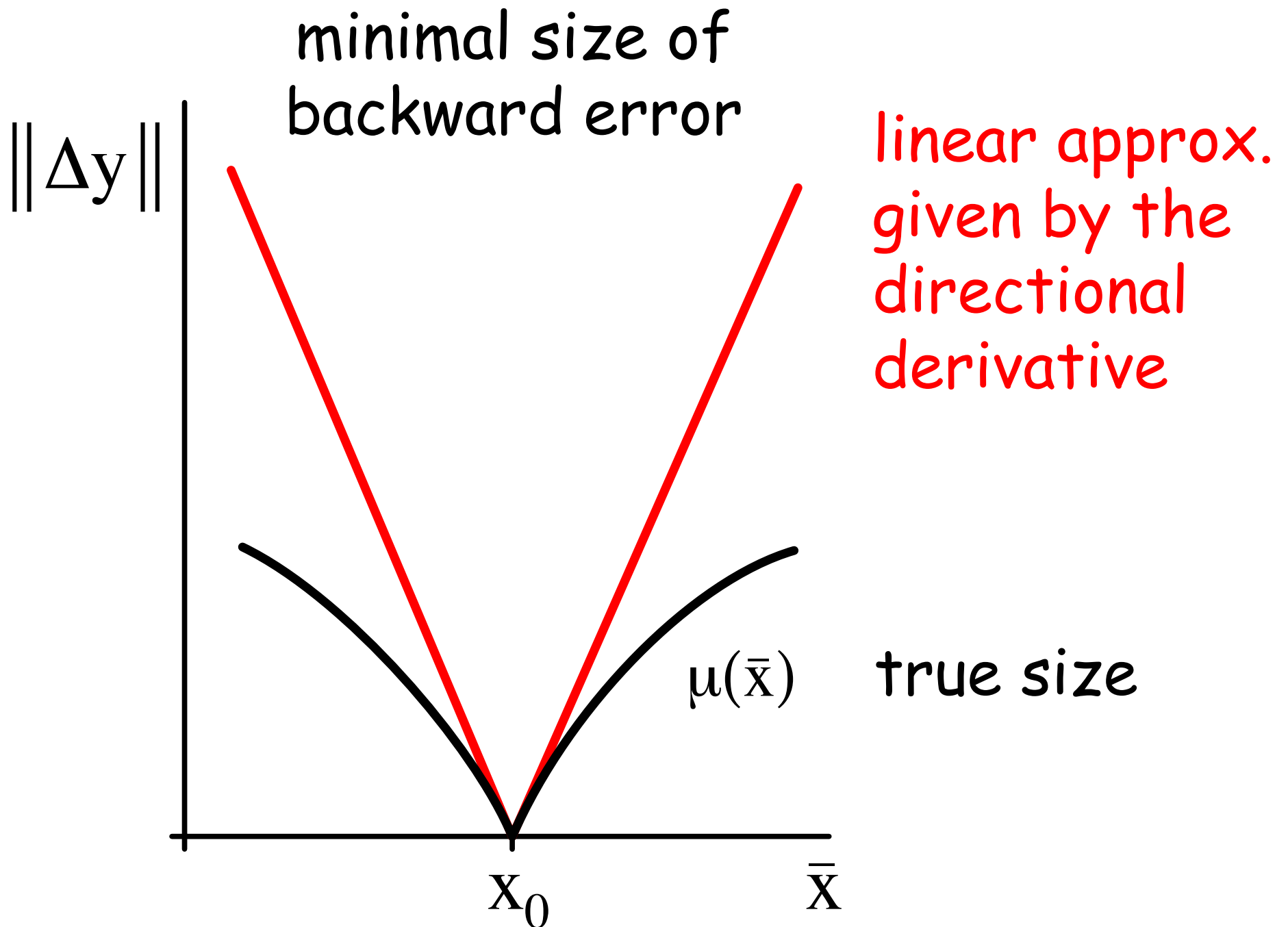
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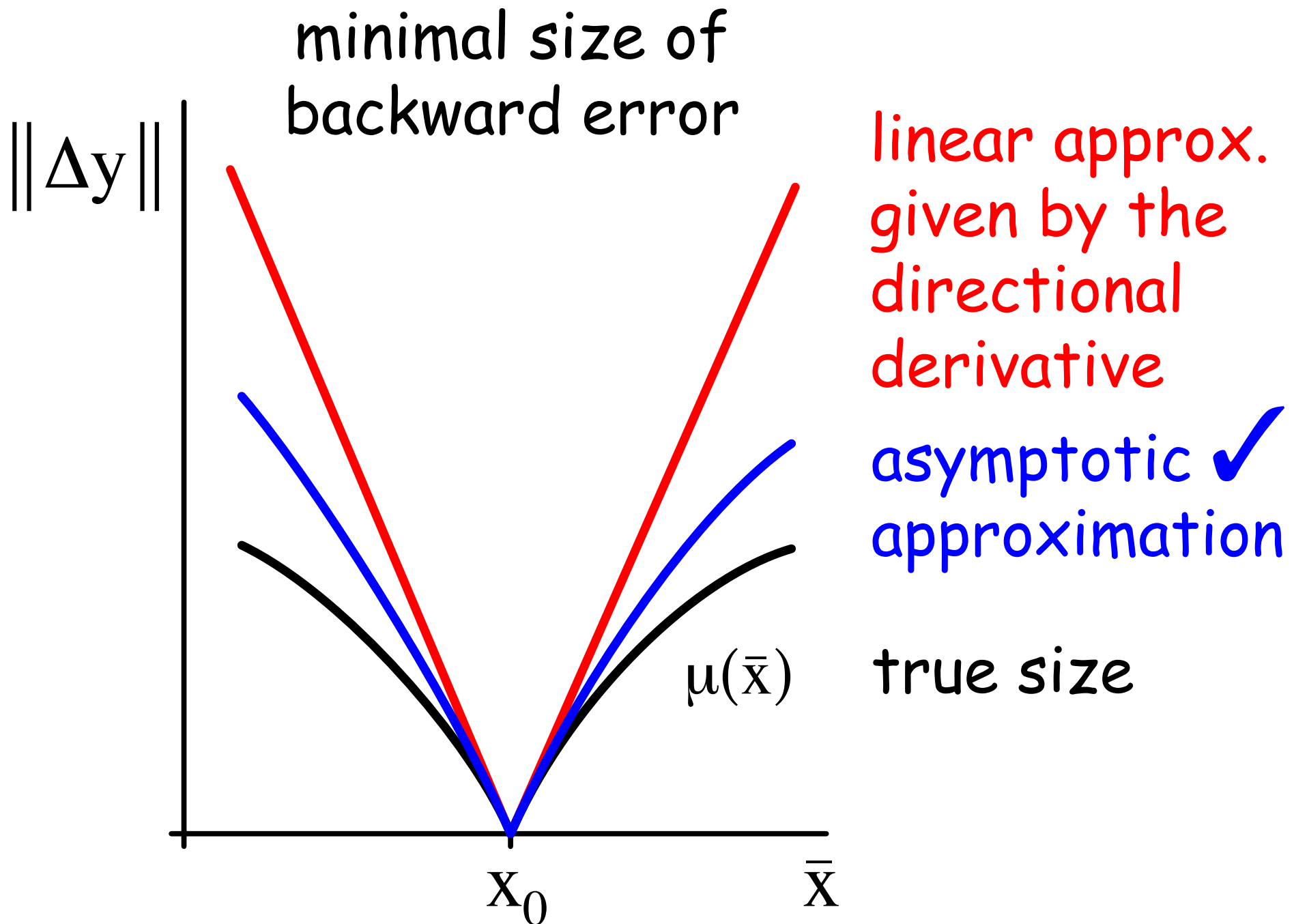
Numerical Examples

Conclusion









If real-valued functions f and g satisfy

$$\lim_{x \rightarrow x_0} \frac{f(x)}{g(x)} = 1$$

then $f \sim g$ at x_0

f asymptotically approximates g , or
 f and g are asymptotically equivalent.

I.e., $\forall \epsilon > 0 \quad \exists \delta > 0$ so that $\|x - x_0\| < \delta \Rightarrow$

$$(1 - \epsilon) g(x) \leq f(x) \leq (1 + \epsilon) g(x)$$

If functions f and g satisfy

$$\mathcal{D}(f - g)(x_0) = 0$$

then at x_0

f differentially approximates g , or
 f and g are differentially equivalent.

- ★ If f, g are asymptotically equivalent at x_0 and if one of f or g is Lipschitz continuous at x_0 , then they are differentially equivalent.

In the minimal size of backward error

$$\mu(\bar{x}) = \min_{\{y' : F(y', \bar{x}) = 0\}} \|y' - y_0\|$$

there are many ways to approximate the constraint

$$F(y', \bar{x}) = 0$$

1. $\mathcal{D}_1 F(y_0, \bar{x}) \Delta y + F(y_0, \bar{x}) = 0$
2. $\mathcal{D}_1 F(y_0, x_0) \Delta y + F(y_0, \bar{x}) = 0$
3. $\mathcal{D}_1 F(y_0, x_0) \Delta y + \mathcal{D}_2 F(y_0, x_0) \Delta x = 0$

Theorem: For residual function F and data y_0 ,

1. if F is continuously Fréchet differentiable,
2. if there is a solution x_0 , i.e. $F(y_0, x_0) = 0$
3. if $\mathcal{D}_1 F(y_0, x_0)$ has full row rank, then

then the minimal size of the backward error

$$\mu(\bar{x}) = \min_{y' : F(y', \bar{x}) = 0} \|y' - y_0\|$$

is asymptotically estimated by replacing the constraint with the first 2 approximations.

If $\mathcal{L} : \mathbb{R}^m \rightarrow \mathbb{R}^p$ maps one space onto another, then

$$\min_{u : \mathcal{L}u = h} \|u\| = \max_{g \in (\mathbb{R}^p)^*} \frac{g(h)}{\|\mathcal{L}^*g\|^*} = \|h\|_{\mathcal{L}}$$

For full row rank matrices \mathbf{J} and 2-norms,

$$\min_{u : \mathbf{J}u = h} \|u\|_2 = \max_g \frac{g^t h}{\|\mathbf{J}^t g\|_2} = \|\mathbf{J}^\dagger h\|_2$$

$h = F(y_0, \bar{x})$ is the residual of the problem

$J = \mathcal{D}_1 F(y_0, \bar{x})$ Jacobian of residual w.r.t. data

$$\mu^{(1)}(\bar{x}) \sim \min_{\Delta y : J \Delta y = h} \underbrace{\|\Delta y\|}_{\text{if 2 norms}} = \|J^\dagger h\|_2$$

★ Nothing depends on, x_0 , the true solution.

★ The estimate can be evaluated.

$h = F(y_0, \bar{x})$ is the residual of the problem

$J = \mathcal{D}_1 F(y_0, \mathbf{x}_0)$ Jacobian of residual w.r.t. data

$$\mu^{(2)}(\bar{x}) \sim \max_g \frac{g^t h}{\|J^t g\|^*} = \|h\|_J \stackrel{\text{if 2 norms}}{=} \|J^\dagger h\|_2$$

- ★ The minimal size of the backward error is asymptotically a norm of the residual.
- ★ The norm is unique.

Linearized equations give asymptotic estimates for the minimal size (in any norm) of the backward error of numerical problem.

1st estimate can be computed for 2-norms by solving a large, sparse LLS problem.

2nd estimate shows the minimal size of the backward error is uniquely determined as a norm of the equations' residual.

Background

Abstract Formulation of the Problem

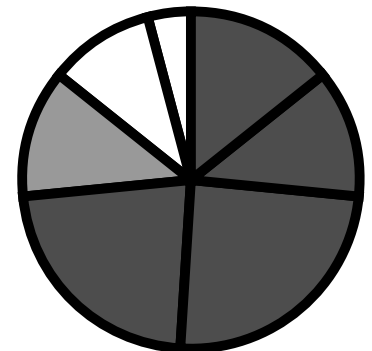
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$$x_0 = \arg \min_x \|b - A_0 x\|_2$$

Find easily computable statistics that are both necessary and sufficient for the stability of a least squares solution. — [Stewart (and Wilkinson), 77]

Exactly minimal size — [Waldén, Karlson, Sun, 95]

$$\mu(\bar{x}) = \min_{\Delta A} \|\Delta A\|_F =$$

$$= \sqrt{\frac{\|\bar{r}\|_2^2}{\|\bar{x}\|_2^2} + \min_i \left\{ 0, \lambda_i \left(A_0 A_0^t - \frac{\bar{r} \bar{r}^t}{\|\bar{x}\|_2^2} \right) \right\}}$$

where $\bar{r} = b - A_0 \bar{x}$

1. Continuously differentiable equations

$$F(A, x) = A^t(b - Ax)$$

2. Any A_0 has at least one solution, x_0

3. $J = \mathcal{D}_1 F(A_0, x_0) =$

$$\begin{bmatrix} e_1 r_0^t & e_2 r_0^t & \cdots & e_n r_0^t \end{bmatrix} - \begin{bmatrix} x_1 A_0^t & x_2 A_0^t & \cdots & x_n A_0^t \end{bmatrix}$$

where $r_0 = b - A_0 x_0$ is the true residual.

Since $A_0^t r_0 = 0$,

$$J J^t = \|r_0\|_2^2 I + \|x_0\|_2^2 A_0^t A_0$$

so J has full row rank provided $r_0 \neq 0$.

Step 2: Form the 2nd Estimate

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The 2nd asymptotic estimate is

$$\begin{aligned}\mu^{(2)}(\bar{x}) &= \| J^\dagger F(A_0, \bar{x}) \|_2 \\ &= \| (J J^t)^{-1/2} A_0^t \bar{r} \|_2 \\ &= \| (\|r_0\|_2^2 I + \|x_0\|_2^2 A_0^t A_0)^{-1/2} A_0^t \bar{r} \|_2\end{aligned}$$

where

$r_0 = b - A_0 x_0$ true least squares residual

$\bar{r} = b - A_0 \bar{x}$ residual of computed \bar{x}

Step 3: Replace $x_0 \rightarrow \bar{x}$

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$$\mu^{(2)}(\bar{x}) = \| (\|r_0\|_2^2 I + \|x_0\|_2^2 A_0^t A_0)^{-1/2} A_0^t \bar{r} \|_2$$

$$\tilde{\mu}(\bar{x}) = \| (\|\bar{r}\|_2^2 I + \|\bar{x}\|_2^2 A_0^t A_0)^{-1/2} A_0^t \bar{r} \|_2$$

This too is asymptotic

$$\lim_{\bar{x} \rightarrow x_0} \frac{\tilde{\mu}(\bar{x})}{\mu(\bar{x})} = \lim_{\bar{x} \rightarrow x_0} \frac{\tilde{\mu}(\bar{x})}{\mu^{(2)}(\bar{x})} \frac{\mu^{(2)}(\bar{x})}{\mu(\bar{x})} = 1$$

For comparison, the exact value is

$$\mu(\bar{x}) = \sqrt{\frac{\|\bar{r}\|_2^2}{\|\bar{x}\|_2^2} + \min \left\{ 0, \lambda_{\min} \left(A_0 A_0^t - \frac{\bar{r} \bar{r}^t}{\|\bar{x}\|_2^2} \right) \right\}}$$

Both Karlson and Waldén, and Gu used formulas equivalent to $\tilde{\mu}(\bar{x})$ to derive other bounds on $\mu(\bar{x})$. Their intermediate results include

- [Karlson and Waldén, 97]

$$\frac{\tilde{\mu}(\bar{x})}{\mu(\bar{x})} \leq \frac{2 + \sqrt{2}}{2} \approx 1.707$$

- when A_0 has full column rank [Gu, 99]

$$1 \approx \frac{\|r_0\|_2}{\|\bar{r}\|_2} \leq \frac{\tilde{\mu}(\bar{x})}{\mu(\bar{x})} \leq \frac{\sqrt{5} + 1}{2} \approx 1.618$$

- so roughly $\mu(\bar{x}) \leq \tilde{\mu}(\bar{x}) \leq 2 \mu(\bar{x})$

- The perturbation theorem can be used to easily derive computable asymptotic estimates for the minimal size of the the backward error of LLS,

$$\tilde{\mu}(\bar{x}) = \| (\|\bar{r}\|_2^2 I + \|\bar{x}\|_2^2 A_0^t A_0)^{-1/2} A_0^t \bar{r} \|_2$$

provided $r_0 \neq 0$ (no restriction on rank of A_0).

- Other results show this is boundedly near $\mu(\bar{x})$.
- And other differential results show any estimate must be of this form.

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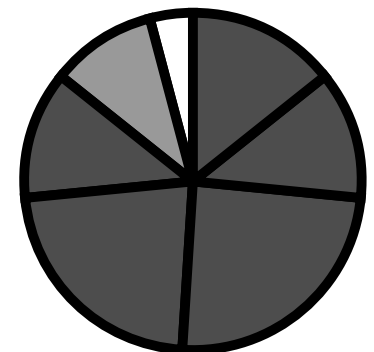
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Evaluating the Estimate $\tilde{\mu}(\bar{x})$

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If a matrix K has full column rank, then the orthogonal projection into $\text{col}(K)$ satisfies

$$\|\mathcal{P}_K v\|_2 = \left\| \left[(K^t K)^{-1/2} K^t \right] v \right\|_2$$

Notice that $\tilde{\mu}(\bar{x}) = \|\mathcal{P}_K v\|_2$ for the choices

$$K = \begin{bmatrix} A_0 \\ \frac{\|\bar{r}\|_2}{\|\bar{x}\|_2} I \end{bmatrix} \quad \text{and} \quad v = \frac{1}{\|\bar{x}\|_2} \begin{bmatrix} \bar{r} \\ 0 \end{bmatrix}$$

Since $A_0 = QR$ is available, use

$$K' = \begin{bmatrix} R \\ 0 \\ \frac{\|\bar{r}\|_2}{\|\bar{x}\|_2} I \end{bmatrix} \quad \text{and} \quad v' = \frac{1}{\|\bar{x}\|_2} \begin{bmatrix} Q^t \bar{r} \\ \dots \\ 0 \end{bmatrix}$$

The zero rows can be discarded, leaving

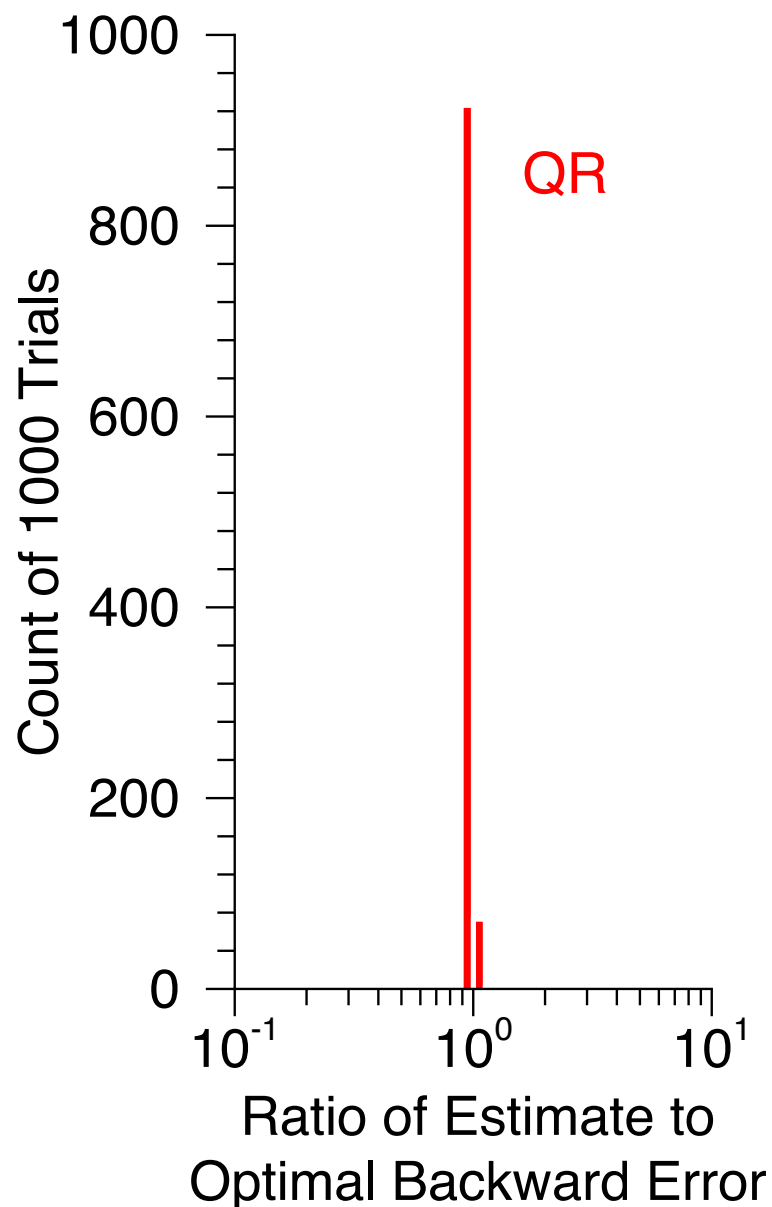
$$K'' = \begin{bmatrix} R \\ \frac{\|\bar{r}\|_2}{\|\bar{x}\|_2} I \end{bmatrix} \quad \text{and} \quad v'' = \frac{1}{\|\bar{x}\|_2} \begin{bmatrix} Q^t \bar{r} \\ 0 \end{bmatrix}$$

It is easy to factor $K'' = Q_K R_K$ using plane rotations [Karlson and Waldén, 97].

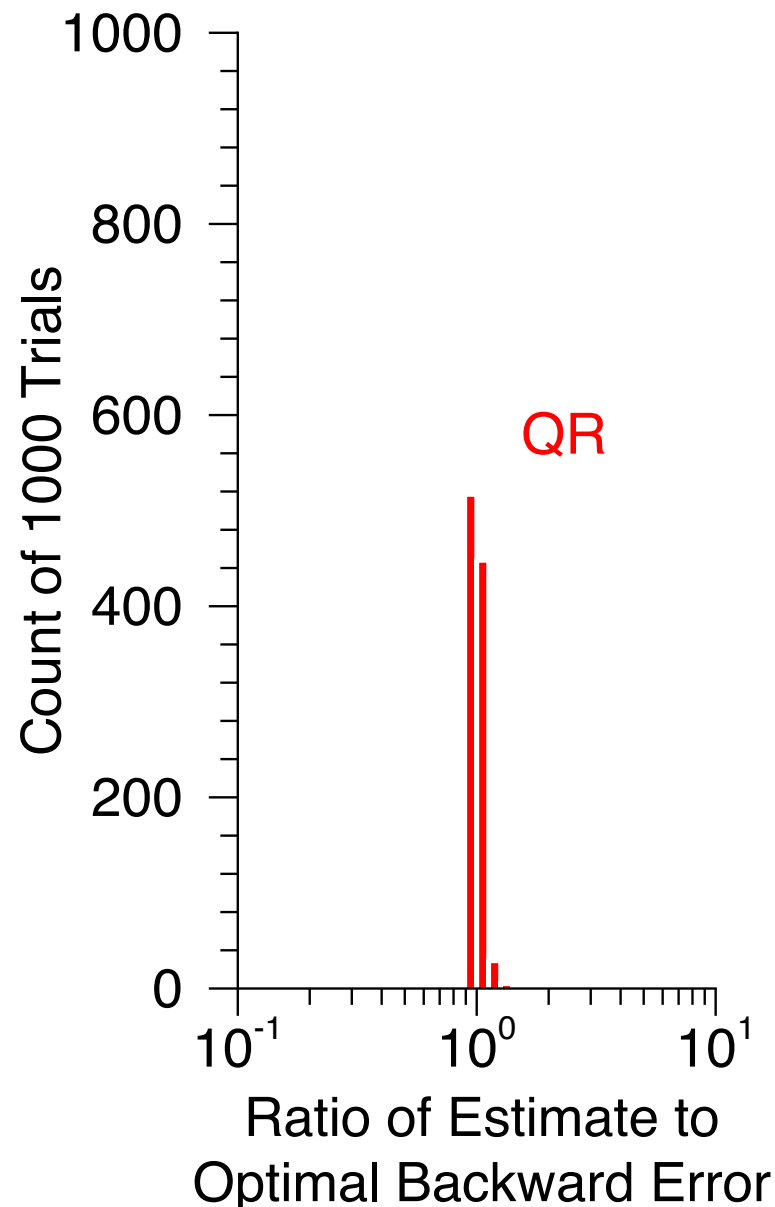
$$\tilde{\mu}(\bar{x}) = \|\mathcal{P}_K v\|_2 = \|\mathcal{P}_{K''} v''\|_2 = \frac{\|Q_{K''}^t Q_A^t \bar{r}\|_2}{\|\bar{x}\|_2}$$

solve LLS by Householder QR	$2mn^2$
form $Q_A^t \bar{r}$	$4mn$
apply $Q_{K''}^t$ to $Q_A^t \bar{r}$	$\frac{8}{3}n^3$
finish evaluating $\tilde{\mu}(\bar{x})$	$2n$

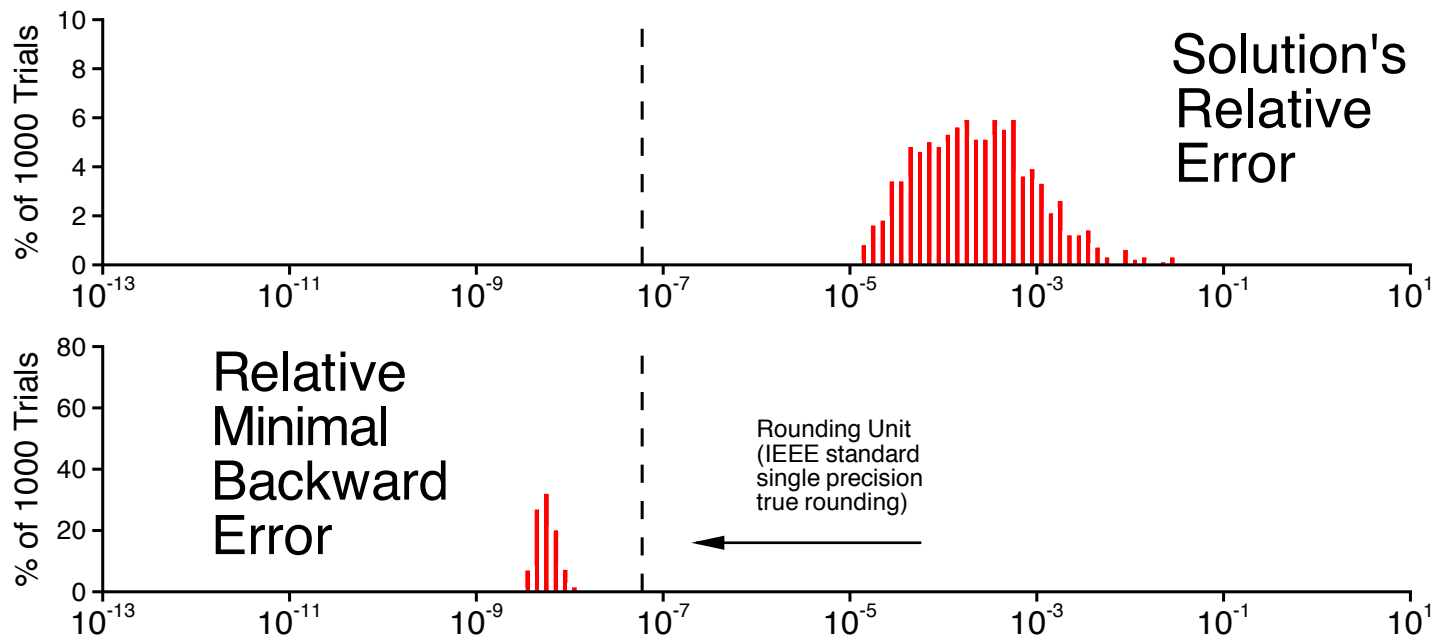
(a) illc1033



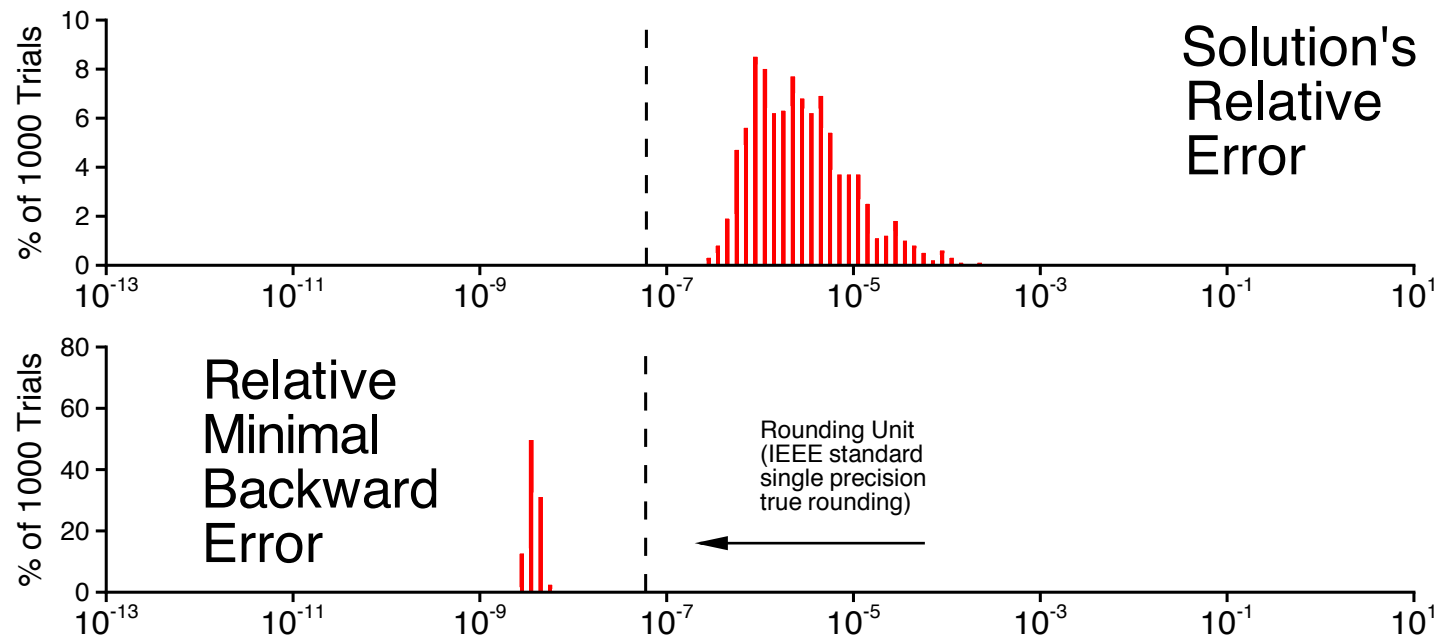
(b) well1033



(a) illc1033



(b) well1033



1. **Accuracy criterion.** [von Neumann, 47]

If the initial data have error $\geq \mu(\bar{x})$,
then \bar{x} solves the problem,
to the extent the problem is known.

2. **Backward stability estimation.**

An \bar{x} with a small $\mu(\bar{x})$ is backward
stable.

3. **Test new algorithms.**

Explore backward stability without having
to do an inverse rounding error analysis.

Background

Abstract Formulation of the Problem

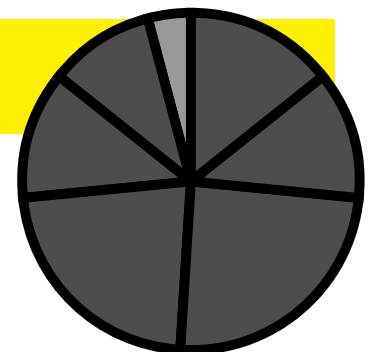
Perturbation Theory of Metric Projections

Asymptotic Approximation

Application to Linear Least Squares

Numerical Evaluation

Conclusion



1. Perturbation theory of metric projections provides asymptotic estimates for optimal backward errors.
2. The estimates can be applied to practical problems such as linear least squares.
3. The estimates for LLS are inexpensive and accurate, answering Stewart and Wilkinson's question.

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Suppose a calculation (program)

1. has inputs (data) y_0
2. has outputs (computed solution) \bar{x}
3. is meant to solve equations $h = F(y, x) = 0$

Do this

1. form the Jacobian matrix, J , of F w.r.t. y
2. evaluate J and h at $y = y_0$ and $x = \bar{x}$
3. use QR or SVD to evaluate $\|J^\dagger h\|_2 \sim \mu(\bar{x})$

Saddle point problem

$$\begin{bmatrix} A & B^t \\ B & C \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

Want backward error to honor the structure

- not separate perturbations to B and B^t
- not perturbations to zeroes in A , B , C

Saddle point problem

$$F(y_0, \bar{x}) = \begin{bmatrix} A & B^t \\ B & C \end{bmatrix} \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix} - \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

Want backward error to honor the structure

- inputs $y_0 = (\text{entries of } A, B, C, b_1, b_2)$
- outputs $\bar{x} = (\bar{x}_1, \bar{x}_2)$

- $J =$ 